Computational Investigations of Mechanisms, Energetics and Dynamics Relevant to CO_2 Sequestration and Capture

L.X. Dang, J.L. Daschbach, V.-A. Glezakou, X. Sun, P.K. Thallapally, and B.P. McGrail

Presented by:

Bruce C. Garrett

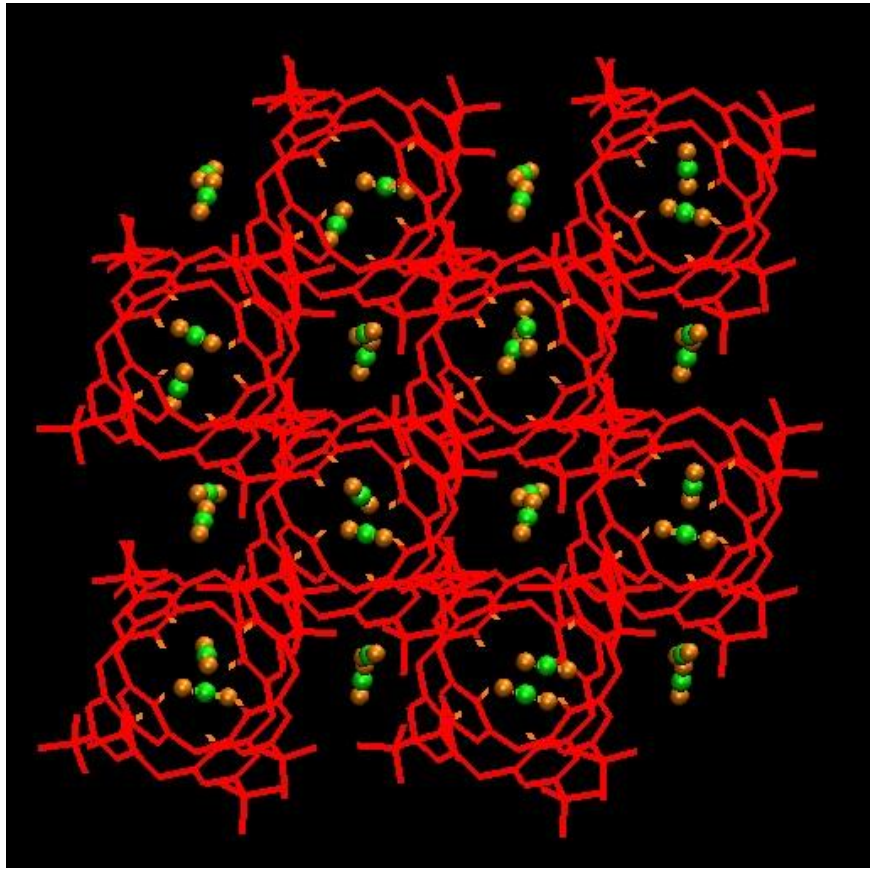
Director, Chemical & Materials Sciences Division

Pacific Northwest National Laboratory

Carbon Capture 2020 workshop, October 5-6, 2009

Computational Studies of Host-Guest Interactions

- Provide a powerful tool that is complementary to experimental studies to probe structures, energetics, and dynamics of host-guest interactions
- Translate knowledge about molecular interaction energies (potential energy surfaces) into thermodynamic and dynamic properties of host-guest complexes
- Yield detailed understanding of factors that control absorption selectivity for inclusion compounds



Pacific Northwest
NATIONAL LABORATORY

Computational Results

- Structures
  - Radial distribution functions are measures of the thermally averaged structures
- Energetics
  - Gibbs free energies provide thermodynamic information related to stability of complexes
- Dynamics
  - Temperature dependence of Einstein frequency (or velocity autocorrelation function) are a measure of thermal conductivity